minerals

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Supplementary Materials

Expanding Family of Litharge-Derived Sulfate Minerals and Synthetic Compounds: Preparation and Crystal Structures of $[Bi_2CuO_3]SO_4$ and $[Ln_2O_2]SO_4$ (*Ln* = Dy and Ho)

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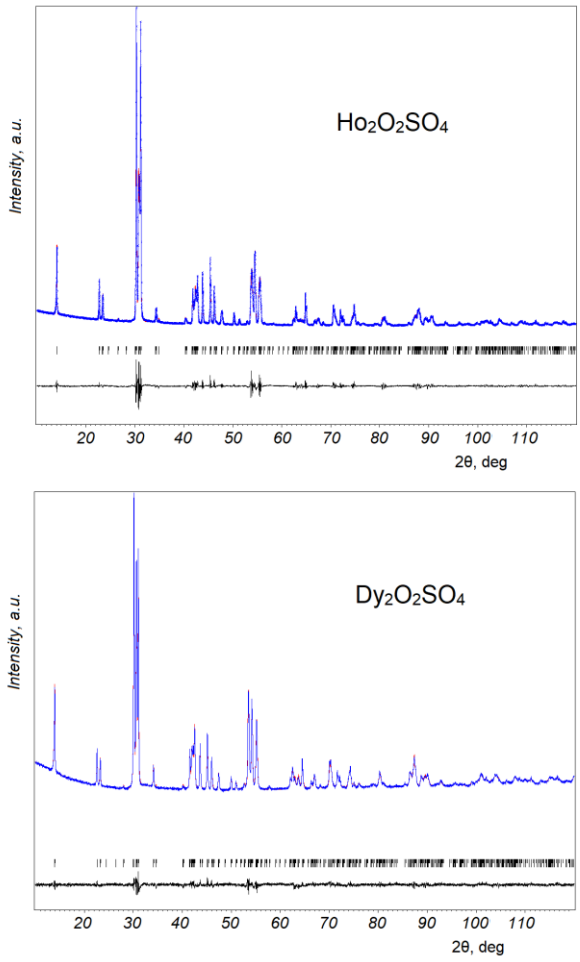

Figure S1. Rietveld refinement plots for $[Ho_2O_2]SO_4$ and $[Dy_2O_2]SO_4$.

Table S1. Coordinates and isotropic displacement parameters (Å²) of atoms in $[Bi_2CuO_3](SO_4)$.

Atom	*x*	*y*	*z*	U_{eq}
Bi1	0.08571(2)	0.54243(3)	0.23864(2)	0.00952(4)
Bi2	0.22857(2)	0.49900(3)	0.56915(2)	0.01026(4)
Cu1	0.08374(3)	0.04136(8)	0.35687(5)	0.00905(10)
S1	0.36572(7)	0.44584(19)	0.89357(11)	0.01223(19)
O1	0.0948(2)	0.2920(6)	0.0462(3)	0.0207(8)
O2	0.0960(2)	0.1502(6)	0.5170(4)	0.0219(7)
O3	0.3786(2)	0.4946(6)	0.8023(4)	0.0181(7)
O4	0.2726(2)	0.4320(7)	0.8319(4)	0.0235(8)
O5	0	0.3013(7)	¼	0.0104(8)
O6	0	0.7855(7)	¼	0.0102(8)
O7	0.16787(17)	0.7780(5)	0.4094(3)	0.0102(5)
O8	0.17049(17)	0.2922(5)	0.3980(3)	0.0107(6)

Table S2. Anisotropic displacement parameters (Å²) of atoms in $[Bi_2CuO_3](SO_4)$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Bi1	0.01101(6)	0.00954(6)	0.00857(8)	−0.00059(4)	0.00636(5)	−0.00037(4)
Bi2	0.00984(6)	0.01064(6)	0.01022(8)	−0.00144(4)	0.00619(6)	−0.00100(4)
Cu1	0.00842(19)	0.00688(17)	0.0097(2)	−0.00032(2)	0.00458(18)	0.00018(14)
S1	0.0173(5)	0.0115(4)	0.0129(5)	−0.0002(3)	0.0118(4)	−0.0008(3)
O1	0.0207(16)	0.0159(14)	0.027(2)	0.0035(13)	0.0153(15)	0.0020(12)
O2	0.038(2)	0.0166(14)	0.0196(19)	0.0056(13)	0.0225(17)	0.0074(14)
O3	0.0241(17)	0.0237(16)	0.0132(18)	−0.0020(12)	0.0149(15)	−0.0050(12)
O4	0.0167(16)	0.0272(18)	0.028(2)	0.0051(16)	0.0143(16)	0.0003(13)
O5	0.0086(16)	0.0082(15)	0.013(2)	0.000	0.0061(15)	0.000
O6	0.0101(17)	0.0085(15)	0.011(2)	0.000	0.0062(15)	0.000
O7	0.0087(11)	0.0101(11)	0.0108(15)	0.0014(10)	0.0056(11)	0.0019(9)
O8	0.0092(11)	0.0078(11)	0.0103(15)	−0.0007(9)	0.0037(11)	−0.0016(9)

Table S3. Coordinates and isotropic displacement parameters (Å²) of atoms in $[Dy_2O_2]SO_4$.

Atom	*x*	*y*	*z*	U_{iso}
Dy1	0.17086(4)	0.5031(5)	0.0846(2)	0.0087(4)
S1	0	0.0388(18)	¼	0.0243(13)
O1	−0.0060(8)	0.2566(8)	0.0964(6)	0.006(1)
O2	0.2484(2)	0.001(4)	0.1208(12)	0.006(1)
O3	0.0935(4)	−0.1489(11)	0.2937(15)	0.006(1)

Table S4. Coordinates and isotropic displacement parameters (Å²) of atoms in $[Ho_2O_2]SO_4$.

Atom	*x*	*y*	*z*	U_{iso}
Ho1	0.17118(7)	0.4968(4)	0.08464(13)	0.0056(6)
S1	0	0.0533(13)	¼	0.0141(15)
O1	−0.0034(5)	0.2701(10)	0.0958(6)	0.0023(12)
O2	0.2464(3)	0.000(3)	0.1242(7)	0.0023(12)
O3	0.0946(4)	−0.1343(11)	0.2985(9)	0.0023(12)